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TECHNOLOGY ASSESSMENT OF RDX PRODUCTION

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Abstract

The known processes for producing RDX were assessed with the goal of identifying the process that would generate the least waste and pollution. It was concluded that the Bachman process employed at Holston AAP is the most economical process for producing RDX and that it probably produces less waste than any other process. It was generally agreed that the entire Holston operation is a very clean one that complies with all federal and state emission standards. In addition, a number of opportunities in which Holston could reduce their wastes were identified. Preliminary assessments of waste and pollution profiles for alternate materials, with emphasis on dual-use materials, were performed.

I. INTRODUCTION

This report summarizes the activities of the Technology and Assessment Task A4, Subtask A: Nitramines of the SERDP Program for Clean, Agile Manufacturing Technology for Propellants, Explosives and Pyrotechnics. Team members are Michael D. Coburn (NMIMT), Charles D. Brumley (Holston AAP), Richard A. Hollins (NAWC), Philip Pagoria (LLNL), Alfred G. Stern (NSWC), Robert B. Wardle (Thiokol), Carolyn Westerdahl (ARDEC). The primary effort of this subtask for FY93 was to study the life cycle waste and pollution profile for RDX production with the goal of reducing waste and pollution by 90%. We were asked to consider improvements in process conditions, equipment, and facilities at Holston AAP that would reduce waste and pollution from the current Bachman process and to determine if any alternate routes to RDX would be more attractive than the Bachman process. In addition, we were asked to perform preliminary assessments of waste and pollution profiles for alternate materials, with emphasis on dual-use materials.

II. APPROACH

A meeting of this task force was held November 30 through December 2, 1993 at Holston AAP. Attendance at the meeting was not restricted to team members, but included members of the Modeling & Simulation Task as well as a number of observers and invited contributors. An extensive tour of the Holston facilities, which included the acetic acid/acetic anhydride and nitric acid plants as well as the RDX production and processing facilities, was conducted. Overviews of the current Bachman RDX and HMX process that is employed at Holston AAP and the Woolwich RDX process that is employed in the United Kingdom were presented by Larry Sotsky (ARDEC). In addition, Larry provided us with a copy of a report by Day & Zimmermann, "RDX/HMX Technology Assessment in Support of Project 5852528", D & Z Project EE 2964-01, 25 May 1983. The Hazardous Waste Minimization (HAZMIN) study at Holston (April 1993) was reviewed by Charley Brumley (a copy of the executive summary of this report is attached as Appendix A). An overview of the GARDEC RDX process

was presented by Bill Lukasavage (GeoCenters) and an economic analysis of this process that was performed by Holston (24 July 1990) was provided by Brumley. Following the discussions related to RDX synthesis, preliminary assessments of waste and pollution profiles for alternate materials were presented.

III. CONCLUSIONS AND RECOMMENDATIONS

A. RDX PRODUCTION

Based upon the tour, Sotsky's presentations, and the Day & Zimmermann report, which validates the conclusions of two earlier key process reports^{1,2}, it was concluded that the Bachman process employed at Holston AAP is the most economical process for producing RDX and that it probably produces less waste than the Woolwich process, the only other process currently used for RDX production. However, both processes should be modeled to verify this conclusion. Larry Sotsky will perform the survey of the current Bachman process and provide the information required to the Modeling & Simulation Task. Norman Paul (DRA, Ft. Halstead) has promised to provide detailed materials and energy balance information on the Woolwich process in current use in the United Kingdom.

It was generally agreed that the entire Holston operation is a very clean one that complies with all federal and state emission standards. The HAZMIN study (Appendix A) identified a number of opportunities in which Holston could reduce their wastes. In addition, it was pointed out that solvent emissions could

be dramatically reduced by installing more efficient condensers.

Suggestions that were posed by team members concerning waste and pollution at Holston are as follows. The idea of using 85% acetic anhydride instead of the 98% should be revisited. Elimination of the final distillation step in the production of 98% acetic anhydride and the resultant sludge would significantly reduce the waste generated by the process. Inject the stack gas ($\text{NO}_x + \text{H}_2\text{O}$) from the nitric acid plant into the NO_2 stream instead of venting it into the atmosphere. Mix the waste RDX/HMX with fuel feed stock for the powerhouse instead of burning it in the open. Sell relatively pure, but off-specification RDX for industrial applications with less stringent specifications.

It was suggested that government regulations and internal Eastman policies be modified so there is more integration. For instance, both facilities make acetic anhydride; furthermore, Holston makes more than it needs, but is not allowed by the government to sell the excess. Site A waste streams could be processed in the Eastman ultramodern water treatment plant instead of being returned five miles to a less modern facility.

Other processes for RDX production that were discussed were the GARDEC process, the Ebele process, the Triazine or TRAT process, and the Wysler process. An economic analysis of the GARDEC process, which first converts formaldehyde and ammonia to pentamethylenetetramine (PMT) prior to nitrolysis to RDX, was performed by Holston in 1990. The results of this analysis indicated that RDX produced by the GARDEC process would be more expensive than that from the Bachman process. In addition, an environmental assessment found the GARDEC process to be less environmentally attractive than the Bachman process because a new chemical (formaldehyde), which is a

¹Hays, Seay, Matern, and Matern, "Technical Assessment of Process Technology for Production of RDX and HMX", May 1980.

²Southwest Research Institute, "Technical Assessment of Known Technology, Domestic and Foreign, for Production of RDX and HMX", August 1980.

regulated, hazardous, carcinogenic material, would be introduced at Holston. Thus, the GARDEC process was not considered for further evaluation at Holston. The Ebele process, which was used to produce RDX at the Bobingen plant of Dynamit A. G., consists of the simultaneous addition of formaldehyde, ammonium nitrate, and acetic anhydride to the reaction vessel such that the temperature of reaction is controlled within the desired range. The yields of RDX are good, but the reaction is catalyzed by a significant amount of boron trifluoride, which is environmentally unfriendly. The Triazine or TRAT process treats acetonitrile or acetamide with formaldehyde to yield 1,3,5-triacetylhexahydrotriazine (TRAT), which is nitrolyzed to RDX with $\text{HNO}_3/\text{P}_2\text{O}_5$, a laboratory source of N_2O_5 . Lukasavage reported that he has never been able to accomplish the latter nitrolysis satisfactorily. The Wysler process is the nitrolysis of hexamine with $\text{HNO}_3/\text{P}_2\text{O}_5$ to yield RDX.

Although the Wysler process has been disregarded over the years because of its use of P_2O_5 to generate N_2O_5 , the recent development of N_2O_5 technology in the U. S. (MUSALL process at Longhorn AAP) and more extensively in the United Kingdom (DRA and ITC) suggests that this process be reevaluated.

B. ALTERNATE MATERIALS

Preliminary life cycle waste and pollution profile estimates for the following alternate or new materials were provided by the team members indicated: ammonium dinitramide (ADN) and 5-nitro-2,4-dihydro-1,2,4-triazole-3-one (NTO) (Stern), 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane (CL-20) (Hollins), 1,3,3-trinitroazetidine (TNAZ) and 2,4-dinitroimidazole (DNI) (Westerdahl, Coburn), and HMX; MUSALL process (Pagoria), GARDEC process (Lukasavage, Westerdahl). In addition, Al Stern provided a comprehensive

overview of N_2O_5 production in the United Kingdom.

NTO and CL-20 have both been produced on the pilot plant scale; thus, reasonable materials balance data exist for modeling. ADN has been prepared on a kg scale and waste streams were estimated. The technologies for producing TNAZ and DNI are not sufficiently established at this time to make reasonable waste stream predictions. The MUSALL HMX process has been piloted at Longhorn AAP and good materials balance information is available. Although the GARDEC HMX process has not been scaled to produce pilot plant quantities, Lukasavage is confident that the process has been optimized to the extent that good materials balance estimates can be made and that HMX can be produced by this process for about the same cost as RDX from the Bachman process.

IV. FUTURE WORK

The initial goal for FY94 will be in-depth assessments of waste and pollution profiles for alternate materials, with emphasis on dual-use materials. The assessments will be provided to the Modeling & Simulation Task to select the most promising alternate materials and processes for optimization and demonstration by members of the network in FY94-97.

Many of the alternate materials under consideration require N_2O_5 for their manufacture. Thus, an assessment of N_2O_5 production will be common to the assessment of waste and pollution profiles of RDX (Wysler process) and these alternate materials, which include HMX (MUSALL and GARDEC processes); ADN and other dinitramide salts; TNAZ; 4,10-dinitro-4,10-diaza-2,6,8,12-tetraoxaisowurtzitane (TEX); 3-nitramino-4-nitrofurazan (NNF) salts; poly(glycidyl nitrate) (PGN); and oxetane monomers. The British, whose N_2O_5 technology is more advanced than

ours, have agreed to cooperate with us in performing this assessment.

Alternate materials under consideration that do not require N_2O_5 in their synthesis include CL-20, NTO, DNI and 1,3,5-triamino-2,4,6-trinitrobenzene (TATB). Both CL-20 and DNI require nitric acid and acetic anhydride for their synthesis, while NTO and TATB require nitric acid.

Substitution of HMX for RDX in both explosive and propellant applications would provide products with improved performance and may be cost effective if HMX could be produced in a more inexpensive and waste/pollution free process. ADN and some of its salts are candidates for minimum smoke propellant applications and may be suitable as gas generators for airbags. Potassium dinitramide is a phase stabilizer for ammonium nitrate in propellant applications. TNAZ is a unique melt-castable explosive with performance comparable to HMX. TEX is an insensitive high explosive (IHE) candidate and the NNF salts are useful propellant ingredients and potential gas generators for airbags under investigation at Thiokol. Poly(glycidyl nitrate) and polyoxetanes are energetic binders for propellants. CL-20 is more energetic than HMX in both explosive and propellant applications. NTO and DNI are both candidates for IHE and airbag applications. A castable TNT/NTO formulation has passed the Air Force sympathetic detonation test and has performance comparable to Composition B. The Air Force is now planning to prepare a high-performance, castable TNAZ/NTO formulation. TATB is the IHE used in nuclear weapons.

In considering the synthesis requirements for all of the above energetic materials, a concept has emerged for a truly agile nitration facility that could be used to prepare all of these materials, assuming that the

non-energetic precursors could be obtained from commercial sources. Such a plant would contain nitric acid, acetic acid/acetic anhydride, nitrogen dioxide/dinitrogen tetroxide (N_2O_4), and electrolytic N_2O_5 facilities, both for production and recovery. Two of the products (CL-20 and TATB) require sulfuric acid and one (TATB) requires ammonia. The latter requirement would be satisfied in the proposed plant because nitric acid production starts with ammonia. The synthesis of ADN and the other DN salts requires acetic anhydride, nitric acid, and N_2O_5 , and the synthesis of CL-20 uses acetic anhydride, nitric acid, and N_2O_4 ; thus, a plant with all the proposed facilities would be necessary to produce these materials. Nitric acid and acetic acid/acetic anhydride facilities exist at the Holston AAP and an electrolytic N_2O_5 facility is in place at the Longhorn AAP, but all of these facilities do not exist at any one plant in the United States. The following scheme is a simplified diagram relating the products to the facilities.

PROPOSED AGILE NITRATION FACILITY

